THE BRING OF GOVERNMED

28 August-1 September 2000

Book of Abstracts

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### Brijuni Conference VII

# Important Problems for the XXI Century \*

August 28 - September 1, 2000 Brijuni, Croatia

Eds.: S. D. Bosanac and N. Došlić

\* This conference is part of the program to celebrate the 50-th anniversary of the Ruđer Bošković Institute

 $Zagreb,\,IRB,\,2000$ 

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### Contents

1.	Program	4
2.	Abstracts	9
3	List of Participants	54

### Monday, 28. August

08.45 - 09.00**Bosanac:** Introductory remarks Chairman: Kleppner 09.00 - 09.40Mainzer: Thinking the future in a global dialogue: Science, technology and society discussion 09.40 - 10.00 Denegri: Large hadron collider project and 10.00 - 10.40physics perspectives 10.40 - 11.00 discussion coffee break 11.00 - 11.20 Chairman: Quack Schopper: Can we understand the ultimate 11.20 - 12.00 structure of matter? - and why should we? 12.00 - 12.20 discussion LUNCH AND BEACH DISCUSSIONS Chairman: Schopper 17.30 - 18.10 Millis: Impact of emerging physics on the prospects for space travel breakthroughs - Warp drive, when? discussion 18.10 - 18.30 Ferenc: The excitement of uncovering the last 18.30 - 19.10 unexplored interval in cosmic electromagnetic radiation spectrum (10-300 GeV) discussion 19.10 - 19.30 **Moore:** Do neutrinos have mass? 19.30 - 19.50 discussion 19.50 - 20.00Chairman: Ferenc 21.00 Openning of poster session

### Tuesday, 29. August

Chairman: Murrell

08.30 - 09.10 Ebbesen: Novel properties in nano

structured materials.

09.10 - 09.30 discussion

09.30 - 10.10 Weiner: Manipulation of matter by optical

forces for the creation of functional

nanostructures

10.10 - 10.30 discussion

10.30 - 10.50 coffee break

Chairman: Toennies

10.50 - 11.10 Suzor - Weiner: The enigma of  $H_3^+$  dissociative

recombination

11.10 - 11.20 discussion

11.20 - 12.10 Murrell: How many molecules in a cup of

tea?

### LUNCH AND BEACH DISCUSSIONS

Chairman: Denegri

17.30 - 18.10 Pichler: Alkali metal vapor:

from ultracold matter to cool brown dwarf

18.10 - 18.30 discussion

18.30 - 19.10 Knop: The future of computing and

networking

19.10 - 19.30 discussion

### Wednesday, 30. August

Chairman: Mainzer	
08.30 - 09.10	Kleppner: The future of quantum physics
09.10 - 09.30	discussion
09.30 - 10.10	Zeilinger: What remains to be done in the foundations of quantum mechanics
10.10 - 10.30	discussion
10.30 - 10.50	coffee break
Chairman: Klemperer	
10.50 - 11.30	Quack: The questions of absolute space and time directions as emerging in biomolecular homochirality and molecular irreversibility: new results and possible answers in the 21st century
11.30 - 11.50	discussion
11.50 - 12.10	Stohner: Parity violating weak nuclear interactions and their influence on rovibrational frequences in chiral molecules
12.10 - 12.20	discussion
12.20 - 12.40	Pavičić: Quantum mechanics for universal quantum computers
12.40 - 12.50	discussion

### LUNCH AND EXCURSION

Chairman: Trinajstić

21.00 White: The role of genetics in the future

of health care

### Thursday, 31. August

Chairman: Leach	
08.30 - 09.10	Luisi: Science facing the question of the origin of life on Earth
09.10 - 09.30	discussion
09.30 - 10.10	Ferris: From space to life; A seamless transition
10.10 - 10.30	discussion
10.30 - 10.50	coffee break
Chairman: <b>Knop</b>	
10.50 - 11.30	Leach: Photostability of prebiotic molecules
11.30 - 11.50	discussion
11.50 - 12.10	Walde: Vesicle as models for protocells: growth and reproduction
12.10 - 12.20	discussion
LUNCH AND BEACH DISC	CUSSIONS

Chairman:	Suzor -	weiller

17.30 - 18.10	Klemperer: How molecules communicate: intermolecular interaction
18.10 - 18.30	discussion
18.30 - 18.50	McCaffery: Energy versus momentum: which determines the outcome of chemical processes?
18.50 - 19.00	discussion
19.00 - 19.20	Klasinc: Trends and cycles in lower tropospheric ozone concentration
19.20 - 19.30	discussion
20.30	GET TOGETHER DINNER

### Friday, 1. September

Chairman: Pichler

08.30 - 09.10 Stwalley: The ultracold frontier for atoms

and molecules

09.10 - 09.30 discussion

09.30 - 10.10 **Toennies:** Molecular spectroscopy in helium

droplets: New microscopic manifestations

of superfluidity

10.10 - 10.30 discussion

10.30 - 10.50 coffee break

Chairman: Pichler

10.50 - 11.30 **Bosanac:** Are we facing the end of science:

reflections on the conference?

2. Abstracts

### Ion-pair satellite bands in heavy alkali dimers: ultracold ion-pair molecule

T. Ban, H. Skenderović R. Beuc and G. Pichler

Institute of Physics, P.O.Box 304, HR-10001 Zagreb, Croatia

We present results of absorption measurements in dense cesium, rubidium and potassium vapor generated in all saphire cells (1,2). New spectral features or satellite bands in the neighbourhood of the second member of the cesium, rubidium and potassium principle series were found. We established no temperature dependence of two peculiar diffuse features in the blue wing of the stronger component (np3/2, n=5,6,7) for potassium, rubidium and cesium, respectively). By applying recent ab initio potential curves at large distances, we were able to construct corresponding difference potential curves with extrema responsible for the observed satellite bands. It appears that these extrema stem from the system of two close lying avoided crossings between ion-pair potential curve and long-range van der Waals potential curves emerging from several neighbouring atomic asymptotes (which also include second excited doublet of the p levels). The uppermost difference potential curve has one minimum and one maximum at very large interatomic distances, which in effect realizes bound electronic state of pure ion-pair character. The implications and aspects of such potentials for the case of ultracold  $K_2$ ,  $Rb_2$  and  $Cs_2$  molecules will be discussed.

<sup>[1]</sup> T. Ban, H. Skenderović R. Beuc and G. Pichler, Europhys.Lett. 48 (1999) 378.

<sup>[2]</sup> T. Ban, S. Ter-Avetisyan, R. Beuc, H. Skenderović and G. Pichler, Chem.Phys.Lett. 313 (1999) 110.

### Clusters: Laboratories to Study Chaos and Regularity

R. Stephen Berry

The University of Chicago

Clusters of atoms, from three to perhaps 10-15 particles, provide vehicles for studying many of the rich aspects of nonlinear dynamics. They are complex enough to be free of the "special case" restrictions that apply only to systems of one or two degrees of freedom, yet are simple enough that we can study their dynamics in considerable detail. One aspect for which clusters are useful is the study of the time evolution of ergodicity. Another aspect that has proven especially interesting is the way different regions of configuration and phase space exhibit different degrees of regularity. Saddle regions on complex surfaces tend to be regions of more regular behavior than regions around minima. This observation has been extended to the study of special properties of the degree of freedom that carries a system across such a saddle, the "reaction coordinate," which, in a suitable canonical (Lie) transform in phase space, preserves its regularity even up to quite high energies, well above the energy at which all other degrees of freedom are chaotic. Moreover in the transformed space, the transmission coefficient, a key parameter in traditional transition-state theory of kinetics, is unity.

### Collision-induced forbidden lines of alkalies atoms

R. Beuc. H. Skenderović T. Ban and G. Pichler

Institute of physics, P.O.Box 304, HR-10001 Zagreb, Croatia

Electric quadrupole allowed transitions from ground S to the first excited D state in the vapors of alkalies have been studied experimentally and theoretically in the past [1-3]. Only recently high quality ab initio potential curves became available [4,5] and this enabled us to model the collision induced shapes of these forbidden lines. In addition to this we performed new high resolution absorption measurements using all sapphire cell [6] in order to obtain absorption coefficient profiles, which could be compared with theoretical shapes.

It is well known that asymptotic transition dipole moments for dipole forbidden S-D transition are extremely small, but sufficiently large for easy observations of forbidden lines at higher atom densities. However, away from the asymptote molecular transition probabilities become large enough and they definitely influence the shape of the relevant line profile.

We shall discuss the results of theoretical calculations, with emphasize on difference potential curves possessing extrema and rapidly changing transition dipole moments. Theoretical shapes of forbidden lines will be compared with experimental absorption profiles, and suggestions for laser induced fluorescence measurements will be given.

Aspects of this work with respect to the detection of ultracold molecules will be discussed for the case of heavier alkali dimers [7].

<sup>1.</sup> K. Niemax, J.Quant.Spectrosc.Radiat.Transfer 17 (1977) 125.

<sup>2.</sup> A. Gallagher and T. Holstein, Phys.Rev.A 16 (1977) 2413.

<sup>3.</sup> R.Beuc: Broadening of dipole forbiden S-D lines in homonuclear and heteronuclear alkali collisional systems, in Spectral Line Shapes, Vol. 3, ed. F.Rostas (Berlin de Gruyter, 1985) pp. 655-6.

<sup>4.</sup> N. Spies and W. Meyer, private communication and to be published.

<sup>5.</sup> S. Rousseau, A. R. Allouche and M. Aubert-Frecon, private communication and to be published.

<sup>6.</sup> T. Ban, H. Skenderović R. Beuc and G. Pichler, Europhy.Lett. 48 (1999) 378

<sup>7.</sup> A. Fioretti, D. Comparat, A. Crubellier, O. Dulieu, F. Masnou-Seeuws, and P. Pillet, Phys.Rev.Lett. 80 (1998) 4402.

### Are we facing the end of science: reflections on the conference?

S. D. Bosanac

#### R. Bošković Institute, Zagreb

The prevailing view today is that the only fundamental problem that needs solution, to have the complete picture of Nature, is to incorporate gravity into the unified theory of fields. This suggests that the end of science is nearing, at least in its fundamental aspect. This view will be challenged in the talk, and the basis will be results that were presented at the conference. It will be argued that despite great strides of science there are a number of very basic fundamental questions that need solution. Are the challenges to answer them indication that something is missing in the formulation of modern physics? And if so is science only at its beginning?

### Unified field theory based on nonlinear electrodynamics

#### Alexander A. Chernitskii

Unified field theory by its sense must describe all particles and its interactions by solutions of unitary nonlinear field model. In this approach the material world is a very difficult exact solution of the model. And elementary particles are solitary solutions or solitons of the model. By this way we can hope to discover new interesting and dramatic effects which will have been defining the progress of civilization.

It is evident that long-range interaction between solitons of such model must have the form of electromagnetic and gravitational interactions which are two known long-range interactions for the material objects. Now we know the effect of induced Riemann geometry in nonlinear electrodynamics (for Born-Infeld model see [1,2]). This effect appear for interaction between solutions such that quick-oscillating wave and solitons behave like light waves and particles in gravitational field.

On the other hand in nonlinear electrodynamics with dyon singularities we have a model of particle with spin [2]. The associated field configuration has two point singularities of electromagnetic field with equal electric and opposite magnetic charges. Such solution is termed bidyon [3]. In Born-Infeld model the bidyon may behave as nonlinear oscillator [2]. With help Lorentz transformation, from the rest oscillating bidyon we can obtain an appropriate moving bidyon solution. It is evident that the moving oscillating bidyon has both particle and wave properties as well as quantum particle.

These properties permit to consider the nonlinear electrodynamics as possible unified field model.

<sup>[1]</sup> A.A. Chernitskii, "Light beams distortion in nonlinear electrodynamics", J. High Energy Phys. 11 (1998) 015, hep-th/9809175.

<sup>[2]</sup> A.A. Chernitskii, "Dyons and Interactions in Nonlinear (Born-Infeld) Electrodynamics", J. High Energy Phys. 12 (1999) 010, hep-th/9911093.

<sup>[3]</sup> A.A. Chernitskii, "Bidyon", Supersymmetry 2000 – Encyclopaedic Dictionary, Eds. P. Favet. J. Gates. S. Duplij, to be published.

### Large Hadron Collider Project and Physics Perspectives

D. Denegri

CERN, CH-1211 Geneve, Switzerland

We present the status of the LHC project, the progress on the construction of the collider, discuss and present the progress on the construction of the large general pourpose detector CMS and give an overview of the physics expectations and discovery potential in Higgs searches, Supersymmetry seraches and SUSY dark matter searches.

### Dissipative Laser Driven Proton Dynamics in Picolinic Acid N-oxide

N. Došlić<sup>1</sup>, J. Mavri<sup>2</sup>, J Stare<sup>2</sup>

R. Bošković Institute, Zagreb, Croatia National Institut of Chemistry, Ljubljana, Slovenia

Laser control of a proton transfer reaction in a small model system embedded in a condensed phase environment is investigated. The two-dimensional model comprises those features of the multi-dimensional potential energy surface of picolinici acid N-oxides which are most relevant for the isomerization reaction. The influence of the remaining intramolecular coordinates as well as of a possible environment is described by a spectral density within the reduced density matrix approach. Different forms of the driving infrared laser pulse are explored putting emphasis on their capability for competing successfully with relaxation processes. The reaction dynamics is characterized by calculating the nonlinear optical response nonperturbatively in the driving field.

### Novel Properties of Nanostructured Materials

T. W. Ebbesen

ISIS, Louis Pasteur University, Strasbourg, France

Materials structured on the nanometer scale can lead to improved and sometimes surprising properties. This can be found both in Nature and more recently in the laboratory. Natural composite materials, such as shells where organic and inorganic components alternate leading to exceptional mechanical properties, are good examples and sources of inspiration. To achieve similar material organization in a systematic manner in the laboratory is one of the challenges in the decades to come. Structure, and preferably composition, need to be controlled at all scales, playing on different types of interactions. It requires bringing together the knowledge from various fields such as chemistry, biology, physics and material science. The potential of nanostructured materials will be illustrated in some detail by our own work on the extraordinary optical properties acquired by metal films if they are simply structured with periodic voids. For instance, subwavelength apertures in such samples will transmit light with an efficiency thousand times larger than theoretically predicted for single holes. These findings and others raise fundamental questions and suggest applications in areas such as near-field optics, sub-wavelength lithography and photonics.

## The excitement of uncovering the last unexplored interval in cosmic electromagnetic radiation spectrum (10-300 GeV)

#### Daniel Ferenc

Physics Department, University of California at Davis, Davis CA-95616

Whenever a new window in the cosmic electromagnetic radiation was opened, important discoveries about the universe followed. Between the lowest energy radio waves and the highest energy gamma rays there is still the last energy interval that has never been probed - the famous "white spot" in cosmic gamma ray radiation, between 10 and 300 GeV. Recent technological advancements, some of them made only for this purpose, will allow us to finally explore this interval. In my presentation I will discuss the key issues in this exciting area, ranging from the recent technological breakthroughs made within the project with their global (spin-off) importance, to the unique opportunity offered, in the contemporary scientific world which is busy with precision measurements of already explored areas -

### From Space to Life: A Seamless Transition

James P. Ferris

NY Center for Studies on the Origins of Life: A NASA Specialized Center for Research and Training, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, NY 12180

The understanding of the origin and occurrence of life in the universe will be one of the primary scientific investigations in the 21st century. What is life? One definition, which is of sufficient generality for application to the possible multitude of incarnations of life in the universe, is that life is a self-replicating system capable of change. Life may have originated on Earth or it may have come from other sites in our solar system. For example, there is a real possibility that life came from Mars or Europa. Large impacters on Mars may have launched Martian life into space and some of this life eventually landed on the earth and seeded life here. Exploration of Mars and Europa may result in the discovery of life, or the remnants of life, on those bodies. Such discoveries could result in a major advance in the understanding the origins of life. The recent discovery of planets outside our solar system provides strong support for the possibility of life elsewhere in the Universe. The search for extra solar planets will be a major research effort in the next 100 years. The discovery of life elsewhere than on the Earth will provide important insight into the significance of life on Earth.

### Future of Research on Intelligence

#### Hermann Haken

University of Stuttgart, Germany

Historically the intelligence of people has been measured by their IQ Now new trends are observed, for instance the usefulness of the IQ is becoming to be doubted and the important role of emotional intelligence is stressed. Intelligence must be judged upon in a more task specific manner. Computers develop abilities that were doubted till few years ago, such as beating of chess grand masters. Deep problems are connected with the computer human interaction. According to the slaving principle of synergetics quickly adaptive systems are enslaved by the less adaptive systems. In this sense, humans are enslaved by computers. But how can we make computers more intelligent? At the same time it appears that emotions must be built in in computational processes. Intelligence will be viewed as as meaningful processing of information, whereby we have to discuss Shannon information, pragmatic and semantic information including the ability of categorization and the resolution of linguistic ambiguities.

Another challenge for intelligence research is provided by the internet that appears to act as a global brain.

At present, we observe a race between seemingly small technological advances that, however, by the multiplication effect of the internet and mass production become highly efficient and the efforts to develop a theoretical frame to cope with emerging new qualitites, such as some kind of superintelligence.

### Trends and Cycles in Lower Tropospheric Ozone Concentration

L. Klasinc, T. Cvitaš, K. Džepina, N. Kezele

Ruđer Bošković Institute, Bijenička 54, Zagreb, Croatia.

Environmental issues are an important challenge for science in the 21. century. The role and fate of ozone in the atmosphere is definitely one of them. Unlike stratospheric ozone which acts as a shield for UV radiation enabling life on Earth's surface and is endangered by production of certain chemicals (Montreal Protocol) ozone in the troposphere is considered a pollutant and health hazard.

Ozone in the troposphere has different sources: diffusion and intrusions from the stratosphere together with lightnings are more important for the free troposphere, whereas photochemistry of nitrogen dioxide is the main source in the planetary boundary layer.

In addition to the formation processes in all these layers, ozone destruction as well as ozone transport is also important. It is indicated that in the past hundred years ozone concentration near the ground has more than doubled and is still rising. Since boundary-layer ozone has to be considered a pollutant, geen-house gas, health hazard, long-term measurements are underway to assess this trend.

We report here various approaches to analysis of 11 years of continuous ozone monitoring data from the station Puntijarka near Zagreb. The site has a rural character (45.90° N; 15.97° E, 980 m a.s.l.) and is representative for the lower troposphere of the whole region.

### How molecules communicate: Intermolecular Interactions.

William Klemperer

Harvard University

We review experiments and calculations on bound and metastable states of molecular complexes. We discuss the geometry of molecular complexes and examine the problem of isomeric forms. A major part of the talk deals with the dependence of the intermolecular potential upon the valence coordinates of the units comprising the complex. In addition to listing successful experiments we review a number of failures.

### The Future of Quantum Physics

Daniel Kleppner

Department of Physics and Research Laboratory of Electronics Massachusetts Institute of Technology

Science is among the most visionary of all human endeavors. Nevertheless, speculations about the future of science are invariably wrong-usually because progress exceeds expectations. A sense of history can provide a perspective for thinking about the future, even though history never repeats itself-at least not in science. At the end of the 19th century, for instance, progress in science was widely celebrated. In retrospect, there should have been widespread dismay because all understanding of matter was empirical. In the 1920s the creation of quantum mechanics suddenly provided a fundamental theory for the structure of matter. That creation transformed science and society in ways that no one could possibly have imagined. Today, at the end of the 20th century, progress in science is being widely celebrated. Nevertheless, it has to be admitted that our understanding of the structure of matter remains fundamentally empirical. What might be the ultimate impact of achieving a much deeper understanding

### The Future of Computing and Networking

Jan Knop

University of Düsseldorf

Are we really at the beginning of the "age of spiritual machines" proclaimed by some authors? Starting from today's state-of-the-art and current trend-setting theoretical or technological approaches the lecture presents some predictions and theses for computing and net-working in the 21st century. As crucial points for future development in this area not only forthcoming evolution steps of processor or internet performance but also completely new services and technologies to be expected in the next three decades are discussed. The overview is concluded by remarks on imaginable long-term progress in information technologies and on possible consequences for human society.

### Non-linear effects in cavity ringdown spectroscopy of the lithium dimer

I. Labazan and S. Milošević

Institute of Physics, P. O. Box 304, HR-1000 Zagreb, Croatia

Cavity ringdown spectroscopy, CRDS [1], is used to measure absorption spectra of dense lithium vapour generated in the heat-pipe oven. Absorption spectra obtained from fitting procedure in time windows of different lengths and placed at different positions across the ringdown decaying curve are presented. Non-linear effects are detected, such as decreasing of absorption with increasing laser pulse energy. Pronounced dips in the line center of strong transitions occur depending on molecular densities, injected laser pulse energies and chosen time window [2]. CRD spectra are compared with integrated cavity output spectra, ICOS [3].

CRDS absorption method is applied on measurements of small absorption coefficients in the spectral region of two-photon transitions. In this case differential equation for the intracavity field intensity becomes non-linear. Absorption spectra around two-photon Li(2S-3D), Li(2S-5D) and Li(2S-6D) transitions and quasiresonant Li(2P-4S) transition are measured. In addition, vibrational-rotational transitions of Li<sub>2</sub>(X  $^{1}\Sigma_{g}^{+}$  -A  $^{1}\Sigma_{u}^{+}$ ) and Li<sub>2</sub>(X  $^{1}\Sigma_{g}^{+}$  -B  $^{1}\Pi_{u}$ ) bands in this spectral regions are identified.

Using CRDS, absorption spectra of lithium and cadmium vapour mixture is measured, in order to observe bound-bound transition of LiCd excimer molecule [4]. Comparing this spectra with absorption spectra of pure lithium vapour we identify narrow intervals of wavelengths in which absorption of  $\text{Li}_2(X^{-1}\Sigma_g^+ - B^{-1}\Pi_u)$  band transition is small or zero. The application of selective wavelength excitation spectroscopy in this spectral windows allows us to discriminate between overlapping  $\text{Li}_2(X^{-1}\Sigma_g^+ - B^{-1}\Pi_u)$  and LiCd bands.

<sup>[1]</sup> M. D. Wheeler, S. M. Newman, A. J. Orr-Ewing, M. N. R Ashfold, J. Chem. Soc., Faraday Trans. 94 (1998) 337-351

<sup>[2]</sup> I. Labazan, S. Rudić S. Milošević Chem. Phys. Lett. 320 (2000) 613-623

<sup>[3]</sup> A. O' Keefe, Chem. Phys. Lett. 293 (1998) 331-336

<sup>[4]</sup> S. Milošević 'Spectral Line Shapes' (A. D. May, J. R. Drummond, and E. Oks, Eds), Vol. 8, Am. Inst. of Phys. Conf. Proc. 328, p.391-405. Am. Inst. of Phys., College Park, MD. 1995

### The Photostability of Prebiotic Molecules

Sydney Leach

Observatoire de Paris-Meudon

I will discuss results on the photostability of some simple prebiotic molecules, as well as aminoacids and nucleic acid bases, which we have studied in the gas phase using synchrotron radiation as excitation source. Formic acid, HCOOH, is an example of a simple prebiotic molecule. It is one of the possible building blocks of biomolecules and it has been observed by radioastronomy in several sites in the interstellar medium (ISM), in particular in regions of massive star formation. It is a general component of ices occurring in the vicinity of embedded high-mass young stellar objects. Its photochemical decomposition products, such as HCO, have been observed in interstellar clouds. Although the ion HCOOH+ has not been observed directly in the ISM, decomposition products such as HCO<sup>+</sup>, which plays an important role in molecule formation in interstellar clouds, and HOCO<sup>+</sup>, have been observed by radioastronomy. The photophysical properties of HCOOH which we have studied in the VUV are thus of direct interest for radioastronomy searches and for exobiology studies. Results on HCOOH, CH3COOH, CH3CN, etc., will be presented. Aminoacids have been postulated to be formed, and have been searched for, in certain astrophysical sites, while abiotic aminoacids have been detected in carbonaceous chondrite meteorites. Determining the nature of the fragmentation products under UV radiation will help in choosing prospective observational sites, as well as providing information on possible mechanisms of formation and destruction of aminoacids in meteoritic materials. Some of the photofragmentation products of glycine, ?-alanine and ?-alanine include species observed in the ISM, e.g. HCNH<sup>+</sup>. We observed marked effects of alanine isomerisation on the photostability and nature of the dissociative ionization products. We have also investigated other aminoacids observed in meteorites, for example ?-amino-isobutyric acid, which is the most abundant aminoacid in the Murchison meteorite, as well as valine and leucine. Preliminary studies on three nucleic acid bases, uracil, thymine and adenine have shown the importance of the reactions in which neutral or ionized HCNO species are formed. HCNO has been observed in the ISM by radioastronomy. These initial laboratory experiments are being extended in order to study in more detail some of the minor products. A comparison will be made between the results of our studies and those of condensed phase species that have been exposed to solar UV radiation in a BIOPAN-1 and BIOPAN-2 experiments fixed to the Russian FOTON-9 satellite. Space radiation exposure experiments planned to be carried out on the International Space Station will be discussed.

### Science Facing the Question of the Origin of Life on Earth

Pier Luigi Luisi

Institute for Polymers, Swiss Federal Institute of Technology, ETH-Zürich

The main assumption in the field of the origin of life is that the early living cells derives from the inanimate matter via a spontaneous process of molecular evolution, namely a gradual increase of molecular complexity and specificity till the onset of the genetic machinery. One of the consequences of this view is that the transition to life can be in principle reconstructed in the laboratory. The lecture will review the conceptual framework and the operational assumptions implicit in these views; and will outline the questions which are still unsolved, both conceptually and operationally, in the pathway of the transition to life. In particular the difficulties inherent in the RNA-world-approach as well as those present in the compartimentalistic view will be presented. Finally the "top-down" and the "bottom-up" approach to the construction of the early cell will be briefly discussed.

### Reaction Mechanism of Ozone Addition to Ethene and its Monohalogenated Derivatives

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The reactions with ozone, beside the reactions with hydroxyl and nitrate radicals, represent the most important tropospheric sink for biogenic and anthropogenic alkenes. For that reason, in the past 40 years a number of studies have dealt with their kinetic and mechanistic aspects. Although the overall kinetics of these reactions is largely known nowadays, there is still a considerable uncertainty regarding their detailed mechanisms and product yields. In this work ab initio CASSCF an CASPT2 methods were employed in studying the reaction mechanisms of ozone with ethene, fluoro- and chloroethene up to the formation of the primary addition product (ozonide). Structural and electronic properties of the reactants, transition states and addition products were determined and discussed. Also given are the analyses of the kinetic parameteres in terms of the simple transition state theory (TST). Finally, in case of the ozone addition to ethene, reaction patth study (IRC) was carried out and led to the determinantion of an approximate structure of the pre-reaction van der Waals complex. Whenever possible, a comparison is made between theoretical and experimental values and these are generally in a good agreement.

### Thinking the Future in a Global Dialogue: Science, Technology, and Society

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The trend towards globalization shows that today knowledge and skills no longer stop at national borders. The worldwide interconnections between science, technology, and society require an understanding of other cultures and ways of thinks. For a long-term safeguarding of the future we need global and multicausal thinking. Multidisciplinary cooperation and internationalization offer enormous opportunities to the individual as well as to society. Basic and applied research provide the necessary knowledge for future generations and for sustainable development respectively. Science works with models which are used to explain contexts as well as to forecast developments. According the scope of topics at the Brijuni conference, questions of forecasting, modeling, and foresight are discussed for the issues of space, material and life sciences. But, besides matter and life, the chief ingredients of the 21st century are information and knowledge. Thus, information and communication technologies are the driving forces towards a global knowledge-based society. Global networking is opening up new forms of information and communication as well as changing our world of work, our cultures and behavioral patterns. These trends and their consequences will be the focal points of a global dialogue.

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### Energy versus Momentum: Which Determines the Outcome of Chemical Processes?

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Recent experiments and their analysis suggests a common mechanism for collision-induced processes from inelastic to reactive collisions. The driving force is the exchange of momentum and is the constant mechanism in a wide range of events. Energy conservation provides the boundaries within which the mechanism may operate and the variation of these from system to system gives great richness to the observed outcomes. The operation of the mechanism and the boundary conditions may be depicted in diagramatic form based on relationships that emphasise the reality of molecular shapes and sizes. In some cases, the boundary conditions force population to focus into very narrow distributions, a situation that can survive many collisions without degradation.

### Molecular Lesion Spectra as Radiation Signatures: Risk Assessment and a Potential Medical Tool

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New post-genomic and proteomic experimental technologies are in process of development. However. a corresponding integrative biophysical modeling of the events along the spatio-temporal path of molecular changes that can make use of that new information seems to be more difficult because it demands a close collaboration between physicists, chemists, biologists and medical professionals. McGlynn and Rupnik (1991) suggested such an integrative approach to the study of post-radiation effects, namely a radiation signature paradigm. Its aim was the protection of populations against radiation damage. The modeling utilizes 1) the new knowledge provided by molecular studies of radiation-matter interactions, particularly databases involving lesions generated in DNA, proteins and bio-molecules as a result of changes in their intercellular and extracellular environments; and 2) newly developing adaptive and genetic models for parallel distributive processing. Using these adaptive models. it is possible to extract and quantify radiation signatures and/or markers, even in rather uncertain and unpredictable conditions. Adaptive models also aid the interpretation of the results. The radiation signatures can provide appropriate lesion sets for real world medicine, and can be used to develop a low-dose, small, personalized monitoring capability for fast radiation exposure estimates.

### Impact of Emerging Physics on the Prospects for Space Travel Breakthroughs

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As new theories and data on natural phenomena emerge, the scientific community works to determine their validity and relevance toward answering such major questions as the age of the universe, the mystery of missing matter, or the coupling of the fundamental forces. Aside from these grand questions, however, there also exists a utilitarian challenge space flight. Presently, space flight is constrained by the fundamental limitations of rocket propulsion. For example, it is presently impossible to send an interstellar probe to our nearest neighboring star within a human life span. These limits cannot be overcome with engineering refinements as they are based on the very physics of rocketry. To revolutionize space flight and enable interstellar voyages, new propulsion physics is required. NASA created the Breakthrough Propulsion Physics (BPP) project to seek further advancements in physics from which such propulsion breakthroughs can eventually be derived - if physically possible. Three visionary breakthroughs are sought: (1) propulsion that requires no propellant mass, (2) propulsion that circumvents existing speed limits, and (3) breakthrough methods of energy production to power such devices. Topics of interest include experiments and theories regarding the coupling of gravity and electromagnetism, vacuum fluctuation energy, warp drives and wormholes, and superluminal quantum effects. Because these propulsion goals are presumably far from fruition, a special emphasis is to identify and support incremental and credible research that will make measurable progress toward these propulsion goals. The latest status of the Project is presented, including descriptions of currently supported research.

### Do Neutrinos Have Mass?

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The neutrino was postulated 70 years ago by Pauli to solve a problem in beta decay and the electron neutrino was experimentally discovered 45 years ago by Reines and Cowen. Today the Standard Model (of High Energy Physics) includes three distinct types of neutrinos. Experimental evidence will be summarized that indicates that these neutrinos can oscillate among themselves and hence have mass. Future experiments will be discussed that will address various questions that are open.

### How Many Molecules in a Cup of Tea?

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Avogadro made his hypothesis in 1811, following earlier proposals by Gay-Lussac that when gases reacted together they did so in simple ratios. The first estimate of Avogadro's number was in 1865, following work of Loschmidt, and since then there have been a wide variety of methods used to improve the accuracy which we can give to this number, and experiments were made by some of the most prominent people in physical science. For their time the experiments showed great originality and were made with extraordinary care.

Avogadro's number, 6.0221367x10<sup>23</sup> is a great example of nearly 200 years developement of physical science.

### Computing the Resistance Distance Matrix

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A novel algorithm for computing the resistance distance matrix is presented. An electrical network is depicted by a graph in which the edges represent units resistor and vertices correspond to junctions in the network. The computation is based on the Laplacian matrix of a graph and auxiliary matrices. The resistance distance matrix is used, for example, to generate the Kirchhoff index for characterizing electrical networks

### Quantum Mechanics for Universal Quantum Computers

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We have recently proved that one can ascribe a logic to neither classical nor quantum bare experimental data. Hence our theories heavily depend on a chosen mathematical model the data fit. For quantum theory this is infinite dimensional Hilbert space which assumes a continuous 3-D space. However, we have also shown that a universal quantum computer cannot use such a theory - it requires finite dimensional Hilbert space and a discrete 3-D space. The latter theory suffices for a perfect simulation of a molecule on a quantum computer. Should we abandon continuum althogether?

#### Diffuse bands of alkali dimers: Detection of ultracold molecules

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In recent few years many efforts have been performed in order to create ultracold molecules and to detect them in their lowest stable states. In the case of alkali dimers ultracold molecules can be formed either in the lowest triplet state, a  ${}^3\Sigma^+_u$  [1] or in the ground state, X  ${}^1\Sigma^+_g$  [2]. Beside Cs<sub>2</sub> and K<sub>2</sub> ultracold molecules, quite recently, ultracold Rb<sub>2</sub> molecules have been detected in their lowest triplet state [3]. Detection scheme of the ultracold triplet alkali molecules is performed via two-photon ionization leading to Cs<sub>2</sub>+ or Rb<sub>2</sub>+. The first step in this ionization process involves absorption of the photons within the well-known diffuse bands of alkali dimers [4].

We have performed a new set of absorption measurements using all sapphire cell filled with potassium, rubidium and cesium at very high temperatures in order to study  $K_2$ ,  $Rb_2$  and  $Cs_2$  diffuse bands at 575, 600 and 710 nm in more details. Using recent ab initio potential curves calculations we shall discuss the origin of the fine structure splitting of these diffuse bands and some additional structures found at very high alkali particle densities.

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# Alkali metal vapor: from ultracold matter to cool brown dwarf stars

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We shall discuss most recent experiments with pure or mixtures of alkali vapors generated at high temperatures and densities in all sapphire cells. A simple absorption spectroscopy supported by the calculations of spectral profiles in which most recent ab initio potential curves were used, provide a mean of understanding of most prominent diffuse spectral features in Cs<sub>2</sub>, Rb<sub>2</sub>, KRb and K<sub>2</sub> dimers.

Some of these spectral features named "diffuse bands" may be used for the detection of ultracold alkali molecules, produced in photoassociation of ultracold atom pair and spontaneous emission. The same diffuse band may be used for the detection of even colder molecules formed by a Raman process in Bose Einstein condensates of rubidium or lithium atoms.

Laser spectroscopy of ultracold and hot alkali atoms and molecules can mutually enrich our knowledge of collision processes in alkali vapors. When alkali vapor is immersed in the atmosphere of hydrogen molecules and helium atoms some interesting spectral line broadening may occur which has a direct application to the atmospheres of cool brown dwarf stars. Future experiments in this interesting field will be discussed in view of the most recent astrophysical findings.

#### The Universality of Mental Processing in Reading

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Competent reading performance of 4th grade Scottish and Brazilian children was compared. The reading performance of the two samples was assessed by a word and non-word test (the words varied in levels of familiarity, regularity and length and the non-words in length). The main objective of the work was the establishment of parameters of efficient reading performance which was taken as reference to the identification of areas of inefficiencies among Brazilian competent readers and also to compare the performance of these children with the performance of the English speaking counterparts to discover the aspects of the reading process that are common to the processing of information regardless of language differences, educational and social-cultural influences and the aspects that are orthography-specific. The main finding of this work is that the theory of English reading processes, can with few exceptions be applied to explain the reading processes in Portuguese. Competent reading in the two languages showed similarities in regard to time processing and error rates for the reading of words and non-words and mainly differed in terms of the generality of the regularity effect and of the rate of letter processing for words and for non-words.

## On the Hosoya Hyperindex and the Molecular Indices Based on a New Decomposition of the Hosoya Z Matrix

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The decomposition of the Hosoya Z matrix into the sum of  $_kZ$  matrices, k=0,1,2,..., is proposed. The  $_kZ$  matrix is based on the independent sets of k edges of the spanning subgraphs generated in the construction of the Z matrix. The Hosoya hyperindex H and a set of structurally related molecular indices  $_kZ$  defined as the sum of all off-diagonal entries in the upper triangle of the Z matrix and the corresponding  $_kZ$  matrices, respectively, are put forward and studied analytically.

The questions of absolute space and time directions as emerging in biomolecular homochirality and molecular irreversibility. New results and possible answers in the 21<sup>st</sup> century

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The three discrete symmetries of nature C (invariance of the hamiltonian under charge conjugation – symmetrical equivalence between matter and antimatter), P (Parity conservation, invariance of the hamiltonian under space inversion) and T (time reversal symmetry) are well known to be fundamentally violated. We discuss the possible relation of this symmetry violation to the observation of prevalence of matter over antimatter in the universe, the prevalence of L-aminoacids and D-sugars over D-aminoacids and L-sugars in the biochemistry of evolution ("homochirality") and the observation of a unique time direction in natural processes. Particular stress will be laid on molecular spectroscopy as a possible experimental approach towards the symmetry violations connected with T and P [1, 2].

Current calculations [5, 4, 5, 6, 7, 8, 10] on parity violation in molecules lead to orders of magnitude larger values than previously anticipated [4]. The consequences for the selection of biomolecular homochirality are discussed.

If time permits, we will discuss CPT symmetry violation and the hypothetical construction of an absolute molecular clock (defining an absolute time direction).

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# Can we Understand the Ultimate Structure of Matter? - and Why Should We?

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During the past 50 years ever increasing accelerators and storage rings have revealed smaller and smaller building blocks of matter. However, recent results indicate that the continuing subdivision of matter in smaller parts comes to an end. The description of matter in terms of ultimate elements and forces between them has to be replaced by other paradigms. These are symmetries which are at the basis of the Standard Model of Elementary Particles. This model has been corroborated mainly by results from LEP (the largest existing research instrument) to an accuracy similar to that of QED. However, there must be 'new physics' beyond the Standard Model. The unification of the forces and the understanding of mass are only two of the remaining riddles. These questions have direct relations to cosmology. The investigation of matter has general and philosophical consequences for our view of the world ('Weltbild'). To penetrate into the microcosmos requires also new techniques which lead to new applications. A few examples will be discussed.

## Diffuse and triplet satellite bands of KRb molecule

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In a hot metal vapor K-Rb mixture spectral phenomena of both  $K_2$  and  $Rb_2$  dimers usually appear together with KRb bands. Sometimes spectral overlaps preclude a clear observations of the satellite bands in the vicinity of the first resonance lines. However, in the case of potassium-rubidium vapor mixture the resonance lines are located within 765-795 nm spectral region, and the very far blue quasistatic wing can be investigated in detail. We found beside K and Rb satellite bands three distinct satellite bands at 730 nm and a single shoulder at 755.5 nm that we asigned to KRb heteronuclear molecule. The interpretation of the KRb satellite bands in this region is very similar to the interpretation of  $K_2$  and  $Rb_2$  satellite bands [1] and was presented in a preliminary form in ref. [2]. This will be further discussed in terms of the recent ab initio calculations of the relevant potential curves [3]. Three diffuse bands of KRb peaking at 568.8, 586.3 and 596.4 were found and asigned to the transitions to the (3) and (4) 3? states. Semiclassical spectral simulation were performed with ab inition potentials and aproximate transition dipole functions. Quite recently Gabbanini et al. [4] have detected ultracold  $Rb_2$  in lowest triplet state by two-photon resonance enhanced ionization at about 600 nm. which is the interval of the Rb<sub>2</sub> diffuse bands. We believe that resonance enhanced ionization using observed satellite or diffuse bands of KRb can be useful in the detection of ultracold KRb molecules. It is expected that KRb will play an important role in future development of multispecies condensates because the KRb system has very favorable Franck-Condon factors for the photoassociation process[5].

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# Parity violating weak nuclear interactions and their influence on rovibrational frequencies in chiral molecules

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Whereas Parity Violation in atomic physics has been well established theoretically and experimentally [1, 2], it is still in the exploratory phase in molecular physics [3]. In this paper, the role of parity violation is discussed from the point of view of molecular physics. As an important consequence of parity violation in molecular physics, an energy difference between enantiomers of chiral molecules is being introduced. This parity violating energy difference also gives rise to a shift in ro-vibrational frequencies between enantiomers in the high barrier limit where parity violation dominates over tunnelling.

While the first quantitative calculations date back two decades [4] an important theoretical discovery has been made by our group in configuration interaction singles excitation (CIS) [5] and most recently Multiconfiguration Linear Response (MC-LR) including complete active space methods (CASSCF) [6]. This increased the calculated parity violating energy difference in typical molecules by more than an order of magnitude. This theoretical discovery led to an increased effort to experimentally verify this effect also in molecular physics. It started out with the first high resolution ro-vibrational assignment of the CF-stretching fundamental in CHBrClF and Fluorooxirane [7, 8]. A recent experimental investigation of a ro-vibrational frequency shift between R- and S-CHBrClF at extremely high resolution [9] achieves a discrimination limit  $\Delta \nu/\nu = 10^{-13}$ . This is still several orders of magnitude less sensitive than needed according to our theoretical investigation of this effect [10]. Subsequent calculations by other groups have confirmed the order of magnitude [11].

We will discuss a general tool to derive ro-vibrational frequency shifts between enantiomers in some chiral molecules which will allow to efficiently look for molecular systems that are promising for the successful experimental investigation of this fundamental symmetry violating effect. We include discussion of multidimensional anharmonic coupling [10].

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#### The Ultracold Frontier for Molecules

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The ultracold frontier has progressed rapidly for gaseous atoms, e.g. with achievement of Bose-Einstein condensation for a number of bosonic atoms and of a degenerate Fermi gas for 40K. typically at temperatures on a nanoKelvin scale.[1]

There are now important efforts underway in many laboratories toward achieving comparable results for gaseous molecules. [2] As first steps, alkali metal diatomic molecules (K<sub>2</sub>, Rb<sub>2</sub> and Cs<sub>2</sub>) have been formed (up to 106/sec.) at microKelvin translational temperatures by photoassociative spectroscopy of ultracold atoms. [3] In addition, hotter milliKelvin molecules have been formed, e.g. by helium buffer gas cooling, by atomic recombination on helium clusters, and by deceleration of dipolar molecules. Also, several varieties of the translationally cooled molecules have been trapped. Recent results and near term prospects for advances in ultracold molecules will be summarized.

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# Exactly Soluble Time-Dependent Potentials in Quantum Mechanics

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A procedure for solving time-dependent Schrödinger equation in an exact form is developed on the basis of exactly solvable time-independent models. With the help of auxiliary time-dependent operators, time-independent models are transformed into time-dependent ones. Some Hamiltonians with corresponding solutions for quantum systems of two coupled equations are constructed in an explicit form. The obtained exact solutions are employed to study nonadiabatic geometric phase and transition amplitudes between levels.

### Molecular dynamics and control in ultrashort laser pulses

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Controlling the dynamics of atomic and molecular processes by means of laser radiation has received much recent attention, with the ultimate goal of controlling the outcome and branching ratios of chemical reactions. Experiments [1] and theory [2] are exploring various complementary approaches, based on the coherence properties of laser light, to analyze or manipulate the motion of electrons and nuclei. The temporal coherence is the most actively explored at the moment, due to the recent strides in the development of femtosecond technology. Pump-probe experiments using sequences of ultrashort pulses to create and control electronic or nuclear wavepackets bring new insight into the timing of molecular processes [1]. Time-dependent simulations of such experiments will be reported, with emphasis on the control of competing ionization and dissociation processes [3]. Extension from isolated diatomic molecules (NaI) to small molecular clusters (NaI.CH<sub>3</sub>CN, CsI. CH<sub>3</sub>CN) will be discussed [4].

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## The enigma of H<sub>3</sub><sup>+</sup> dissociative recombination

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The molecular ion  $\mathrm{H}_3^+$ , a generous proton donor, has long been considered as a building block of interstellar chemistry and star formation. It has been discovered only recently (by infrared absorption) in interstellar dense [1] and diffuse [2] molecular clouds. However, its main destruction process in diffuse interstellar medium, the dissociative recombination :

 ${
m H_3^+} + {
m e}$ ?  ${
m H_3^+} + {
m H}$ ,  ${
m H}$  +  ${
m H}$  +  ${
m H}$  which has long been an enigma for experiments, is still so for theory and for astrophysics. ? The experimental value for the rate of this reaction at low energy has ranged over orders of magnitude, depending on the method used for its measurement. The most recent experiments using ion storage rings [3] converge towards a relatively fast rate ( $10^{-7}$  cm<sup>3</sup>s<sup>-1</sup> at 300K, for ground state ions).

With such a fast rate, it is very difficult to explain the large abundance of H3+ ions observed in diffuse interstellar clouds, where it is mainly destroyed by dissociative recombination, due to the high density of electrons.

On the theoretical side, time-dependent 2D calculations [4] confirm the experimental results at high energy as well as the observed predissociation rates of H3 Rydberg states [5]. However, the value for low-energy DR cross section, deduced from the predissociation rates by an extrapolation procedure, is about 4 orders of magnitude lower than the measured one. A simulation based on multichannel quantum defect theory suggests that an indirect non-adiabatic process may prevail in this case, due to resonant capture into Rydberg series or "closed channels". We are also exploring possible 3D effects which could enhance the indirect process.

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# Inelastic He-atom scattering from surfaces: Is there a structure in the multiphonon "background"?

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We show that the multiphonon backround observed in the time-of-flight (TOF) spectra of He-atoms inelastically scattered from surfaces can in certain regimes show pronounced structures. These structures look like the one-phonon creation/destruction events and can be mistakenly interpreted as such. On the example of He-¿Xe(111) scattering, we interpret these structures, clearly observed in the experimental TOF spectra, as the double convolutions of the Z-polarized surface phonon density of states. The density of states, being (almost) singular at the edge of the surface Brillouin zone, when convoluted with itself indeed looks like a one-phonon emission/absorption TOF peak. Therefore, we call such structures two-phonon deceptons. The precise calculations combining the slab lattice dynamical approach to the calculation of surface phonon dispersions and polarization vectors and the quantum formalism of multiphonon scattering are shown to reproduce the experimental data in all of their aspects.

# Probing "Superfluidity" at the Atomic Level via Infrared Spectroscopy of an OCS Molecule inside 4He-Droplets

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Large  ${}^{4}\text{He}$ ,  ${}^{3}\text{He}$  or mixed droplets with  $10^{3}-10^{4}$  atoms are readily produced in nozzle beam expansions of the cold gas. Their mean sizes, size distributions and densities have all been measured. On passing through a gas filled pick-up cell they readily absorb one or several molecules or mixtures of atoms and molecules, which may agglomerate in the interior to complexes. Heliophobic species such as the open shell alkali atoms and the alkaline earth atoms remain at the surface, whereas closed shell atoms and molecules, which are heliophilic, reside in the interior of the droplets. Embedded heliophilic molecules and van der Waals complexes have been shown to exhibit sharp spectral features in the infra-red, visible and UV by observing the depletion in droplet size resulting from the evaporation following photon absorption [1]. In the vibronic spectra of organic molecules the phonon wing is separated by a gap from the sharp zero phonon lines thereby providing direct evidence that the droplets are superfluid [1]. The well resolved rotational lines in the infrared indicate, moreover, that molecules such as OCS rotate virtually without friction but with about a factor 3 greater moment of inertia. The rotational line intensities indicate droplet temperatures of 0.37 K for pure <sup>4</sup>He droplets and 0.15 K for both pure <sup>3</sup>He droplets as well as for mixed <sup>4</sup>He/<sup>3</sup>He droplets with an inner <sup>4</sup>He cluster core. The free rotations have been shown to be a new microscopic manifestation of superfluidity [2]. With the aim of understanding the increase in the moments of inertia recent spectroscopic experiments have been designed to study in detail the local interactions of the molecule with the first shell of He atoms. By adding one-by-one H<sub>2</sub>, D<sub>2</sub> or HD molecules, which replace the first shell atoms, details on their structures, dynamics and exchanges with the other atoms in the superfluid have been obtained. Large (OCS)- $(pH_2)_{15}$  clusters have also been created inside the droplets and have been observed to undergo a transition to a superfluid state on cooling from 0.38 to 0. 15 K [3]. Other clusters grown inside He droplets appear to have unusual structures not found in gas phase expansions [4].

These experiments illustrate how inside He droplets new exotic states of low temperature matter can be produced with sizes intermediate between the molecules and small clusters studied in gas phase spectroscopy and the macroscopic systems characteristic of low temperature physics. The new technique thus provides new perspectives for both of these mature fields.

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### Vesicles as Models for Protocells: Growth and Reproduction

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If one assumes that life originated on Earth, then this happened about 4.0 - 3.5 billion years ago. The oldest known fossils of living organisms are about 3.5 billion years old. Nothing is known about the very first living systems and their precursor structures. It is, however, generally accepted that one important characteristic property of all living systems is the presence of compartments. There is no life today without cellular compartments, which allow a separation of an internal organization from the environment. Lipid vesicles resembling the basic structure of the lipid matrix of contemporary biological membranes are currently considered as reasonable models for the precursors of the first living systems. Lipid vesicles - also called liposomes or simply vesicles - are formed in aqueous solution upon dispersing a bilayer-forming amphiphile (often just called lipid); they are spherical structures containing an aqueous interior and one (or several) closed lipid bilayers which represent the boundary of the vesicles. The diameter of vesicles can vary between about 20 nm and 0.1 mm or more, covering the sizes of biological cells. Vesicles form from contemporary phospholipids present in biomembranes, such as phosphatidylcholine, or from mixtures of as simple chemical substances as linear fatty acids and the corresponding carboxylates. In this latter case, the kinetics of vesicle formation, vesicle growth and reproduction has been studied, in particular using cis-9-octadecenoic acid and cis-octadecenoate (oleic acid and oleate). Vesicles composed of oleic acid and oleate can be prepared directly from oleate micelles or from oleic anhydride through an alkaline hydrolysis, a process which is autocatalytic and leads to vesicle formation, growth and reproduction.

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# Manipulation of matter by optical forces for the creation of functional nanostructures

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Since the development of the transistor in the latter half of the 20th century, the trend in device development has always been to miniaturize fonctional structures starting from macroscopic materials. Even at the finest limits of this approach the wave properties of matter have been ignored. The 21st century will usher in the era of switches, gates and material waveguides and circuits starting from individual atoms; cooled, confined, and focused by miniature static and dynamic electromagnetic fields. The the de Broglie wavelength will replace the optical wavelength as the limit of spatial figure definition. This talk will dicuss the basic physics, limitations, and potential developments of this regime below the optical diffraction limit.

#### The role of genetics in the future of health care

Jonathan White

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Sequencing of the human genome will bring together life science and information science to create a new force that will change the course of human health, politics, culture and perhaps even morality forever. These changes will be wrought by the rapid ability of industry and government to identify and exploit new information. Clinical geneticists have already begun to show that response to drugs can depend upon an individual's genotype. Whilst this may expedite drug development and lead to more efficacious and safer therapies, these benefits will be realized by targeting the drug to a more restricted patient population. Can private industry afford to do this? Who will pay for non-cost-effective therapies? Will private insurance companies begin to stratify premiums based upon genotype? We are poised to be able to predict and possibly prevent many human diseases through environmental and therapeutic strategies. However, will society tolerate this? How do we keep a balance between serving individuals' health needs without invading their privacy by analyzing the phenotypic consequences of their genomic sequence? My talk will briefly review the technological status of pharmacogenomics and explore the potential applications of this information to human health care. I will also raise some of the intriguing consequences of genome sequencing such as pharmaceutical market fractionation, changes in intellectual property ownership, new demands on pavers and finally the ethical implications of the technological revolution we are all now living through.

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